

Ethylbenzene
100-41-4 | DTXSID3020596

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.95e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.23e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

Image not found

Bromocyclohexane

Measured: 5.08e-03

Predicted: 2.15e-03

Image not found

1,4-Dibromobutane

Measured: 1.62e-03

Predicted: 2.55e-03

Image not found

1,3,5-Cycloheptatriene

Measured: 6.73e-03

Predicted: 4.23e-03

Image not found

Bis-(2-chloroethyl)sulfide

Measured: 4.32e-03

Predicted: 3.70e-03